



LAWRENCE
LIVERMORE
NATIONAL
LABORATORY

LLNL-TR-551211

A Summary of MAGE: A Method for Estimating the Maximum Possible Chemical Energy Content of UCG Product Gas per Unit Area for a Multistrata Coal Zone

E. Shafirovich, D. W. Camp

April 23, 2012

Disclaimer

This document was prepared as an account of work sponsored by an agency of the United States government. Neither the United States government nor Lawrence Livermore National Security, LLC, nor any of their employees makes any warranty, expressed or implied, or assumes any legal liability or responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights. Reference herein to any specific commercial product, process, or service by trade name, trademark, manufacturer, or otherwise does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States government or Lawrence Livermore National Security, LLC. The views and opinions of authors expressed herein do not necessarily state or reflect those of the United States government or Lawrence Livermore National Security, LLC, and shall not be used for advertising or product endorsement purposes.

This work performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344.

A Summary of MAGE: A Method for Estimating the Maximum Possible Chemical Energy Content of UCG Product Gas per Unit Area for a Multistrata Coal Zone

LLNL-TR-551211

Evgeny Shafirovich

David W. Camp

Lawrence Livermore National Laboratory

February 28, 2012

LLNL-TR-551211

This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under contract DE-AC52-07NA27344. Lawrence Livermore National Security, LLC



Disclaimer

This document was prepared as an account of work sponsored by an agency of the United States government. Neither the United States government nor Lawrence Livermore National Security, LLC, nor any of their employees makes any warranty, expressed or implied, or assumes any legal liability or responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights. Reference herein to any specific commercial product, process, or service by trade name, trademark, manufacturer, or otherwise does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States government or Lawrence Livermore National Security, LLC. The views and opinions of authors expressed herein do not necessarily state or reflect those of the United States government or Lawrence Livermore National Security, LLC, and shall not be used for advertising or product endorsement purposes.

Auspices Statement

This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory in part under Contract W-7405-Eng-48 and in part under Contract DE-AC52-07NA27344.

Underground coal gasification (UCG) has the potential to extract energy from unmineable coals in a form of syngas with no CO₂ emissions. The selection of potential sites for UCG, however, is a complicated process that involves consideration of various scientific, technological, and economical issues.

The present report describes a new method for estimating the upper bound on the chemical energy content of UCG product gas per square meter of land area. The product gas would have about this much chemical energy content if there were no water influx, no roof collapse or spalling above the coal zone, no heat lost to the surroundings, no gas losses to the surroundings, and 100% conversion of the coal to produced gas products. This method can particularly be used for comparison of different regions and selection of locations that potentially may provide the highest amounts of energy in the form of UCG product gas. Note that other factors such as geomechanical, physical, and hydrological properties of coal and rock, seam dip, proximity of aquifers, surface infrastructure (e.g., mines, cities, power plants, pipelines), land cost, etc., should also be considered in the site selection process.

It is commonplace in the coal industry to arrive at a summed energy content of multiple coals seams by summing over the seams of interest the product of the as-received coal heating value, times an estimate of the coal density, times the thickness of the seam to produce a total heating value on an areal basis (MJ per m² of land area). The method described in this report more accurately fits the energy balance for underground coal gasification in that it takes into account the energy required to heat the coal ash, coal moisture, parting minerals, partings moisture, and product gas to their final temperature in a UCG operation.

We call this value MAGE, for Maximum Areal Gas chemical Energy in the product gas from a zone containing one or more coal seams.

The estimates for a specific coal basin are based on the information obtained from numerous boreholes. For each borehole, we usually know the depths of all minerals and coals, i.e., in fact we know the thicknesses of all the layers under the surface along the borehole. The coal-containing layers are typically characterized using proximate analysis, which provides weight percentages of moisture, ash, volatiles, and fixed carbon (the sum of these components is equal to 100 %). Each such layer is also characterized by the lower heating value (*LHV*), which constitutes the combustion enthalpy of the material at 25°C minus the latent enthalpy of water vaporization. Often, the layer density is also known.

The lower heating value of the coal (*LHV_c*) is often used for comparison of mined coals. In the case of UCG, however, it is more appropriate to use the lower heating value of the product gas (*LHV_g*). If carbon reacts with oxygen and steam with no energy loss, *LHV* of the obtained gas mixture is equal to that of carbon. This is explained by the conservation of energy (for example, the energy obtained from hydrogen combustion compensates for the energy that needs to be spent for hydrogen formation). The UCG process involves some inherent energy losses that have to be subtracted from *LHV_c* in the estimates of *LHV_g*. Three major mechanisms of energy losses in the coal layer during UCG, accounted for in the present estimate, are:

- Vaporization of water contained in the layer and heating the obtained steam to the product gas temperature (T_g , defined later)
- Heating ash or any other solid remained in the layer to the rubble temperature (T_r , defined later)
- Heating the dry gas products to T_g

An additional energy loss occurs due to heat transfer to the rock layers located between coal layers. As noted above, heat loss to the surroundings is neglected. Often, however, the parallel coal layers are separated by relatively thin layers of rock. The UCG reactor size may exceed the thickness of a single coal layer if the separating rock layer collapses during the cavity growth. In this case, the rock layer will consume the energy for:

- Vaporization of water contained in the layer and heating the obtained steam to T_g
- Heating rock to T_r

In the estimates, such thin layers of rock can be treated as the coal layers with zero LHV_c and no gas products (except for steam). Thus the formula for calculating LHV_g of the UCG product gas from a single coal or rock layer is:

$$LHV_g = LHV_c - (h_{st} - h_w) \cdot mf_w - c_{p\,m} \cdot (T_r - T_o) \cdot mf_m - c_{p\,g} \cdot (T_g - T_o) \cdot mr_g \quad (1)$$

where h_{st} is the enthalpy of steam at T_g , h_w is the enthalpy of liquid water at T_o , $c_{p\,m}$ is the average specific heat of mineral (ash or rock), $c_{p\,g}$ is the average specific heat of product gas, T_o is the initial temperature of coal and rock, mf_w is the mass fraction of water in the layer, mf_m is the mass fraction of mineral (ash or rock) in the layer, and mr_g is the mass ratio of the dry product gas to the coal. The latter parameter is determined by the formula:

$$mr_g = mf_c \cdot (1 - mf_w - mf_m) \cdot \frac{M_g}{M_c} \quad (2)$$

where mf_c is the mass fraction of carbon in dry ash-free coal, M_g is the molar mass of the product gas, and M_c is the molar mass of carbon. Note that for a rock layer, Eq. 1 produces a negative value, which means that the layer does not generate any chemical energy (product gas) and only consumes energy.

The maximum areal gas energy of the layer is determined by the formula:

$$AE = \rho \cdot \delta \cdot LHV_g \quad (3)$$

where ρ is the density of coal or rock in the layer and δ is the thickness of the layer.

Note that the dimension of AE is the unit energy per unit area, e.g., MJ/m².

In Eq. 3, the thickness, δ , is the *vertical* thickness, i.e., the difference between the bottom depth and the top depth of the layer along the borehole. Here we neglect a potential effect of coal seam dip (which is often unknown). For high dip angles, more careful considerations will be needed. During calculations, the operator selects a series of adjacent layers that could be considered as a single UCG reactor. It is recommended that the bottom and top layers consist of coal and the interior rock layers are sufficiently thin to be collapsed during UCG. The maximum areal gas energy of the potential UCG reactor is determined as the sum of AE values of all the layers from the top to the bottom:

$$AE_R = \sum_{i=1}^n AE_i \quad (4)$$

The parameters mf_w and mf_m , and LHV_c are typically known for each coal-containing layer. For rock layers, $LHV_c = 0$, while the values of 0.15 and 0.85 can be assumed for mf_w and mf_m , respectively. The parameter mf_c has also to be known. If it is unknown, typical content of carbon in dry ash-free coal for the specific type of coal (e.g., lignite) can be used.

The product gas temperature, T_g , is defined as the temperature of gas at the bottom of the production well, which can be considered as the exit of the UCG reactor. It is assumed that the energy required for heating gases (including steam) to higher temperatures, that take place in some places inside the UCG reactor, is not lost and is stored as part of a chemical energy of the product gas. Based on previous UCG experience, it is recommended to assume that both T_g and T_r are equal to 500°C. The initial temperature of coal or rock, T_o , is equal to 25°C.

The estimate requires knowledge of the product gas composition, which in general is dependent on the location (e.g., increasing the depth leads to increasing methane content) and injected gas (air vs. oxygen). For simplicity, however, it is recommended to assume some specific gas composition, which is expected for most locations if the same injected gas (e.g., oxygen) is used, for example, 35% H₂, 11% CH₄, 11% CO, and 43% CO₂.

The enthalpies of steam h_{st} and liquid water h_w are determined from steam tables. The specific heat of the product gas, $c_{p,g}$, is determined by averaging the specific heats of the individual gas components at T_o and T_g and applying the formula for the specific heat of a gas mixture. It is assumed that the specific heat of mineral $c_{p,m} = 1$ kJ/kg/K.

If the layer density is unknown, reasonable assumptions can be made (e.g., the density of lignite is 1400 kg/m³ and the density of clay is 1800 kg/m³). Note that the density for the actual (wet) material should be used.